Exploring TeraHertz Laser Design through High Performance Computing

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*** PI of Allocated Project**

**** CIs Allocated Project**

What is TeraHertz radiation?

- TeraHertz radiation is electromagnetic radiation in the 1E12 Hertz frequency range.
- TeraHertz radiation has been historically difficult and expensive to generate in comparison with lower microwave, and higher infrared/optical sources.
- There are two primary philosophies for generating electromagnetic radiation including the use of semiconductor technology
  - Extending microwave electronics to higher frequencies
    - For example oscillating circuits based on high speed electronic devices are typically limited to below 0.3 THz (300 GHz).
  - Extending optical/infrared technologies to lower frequencies
    - For example the semiconductor laser is limited to above 30 THz
  - There is a gap where no semiconductor technology can efficiently convert electric power into electromagnetic radiation

Electromagnetic Spectrum

Wavelength	Wavelength	Wavelength	Frequency	Frequency	Wavenumber	Energy	Temperature	Description
meters	cm	nm	Hz	THz	cm-1	meV	Kelvin	
10.00	1000.00	1.00E+10	3.00E+07	3.00E-05	6.28E-03	1.24E-04	1.44E-03	VHF begins
7.00E-02	7.00	7.00E+07	4.29E+09	4.29E-03	8.98E-01	1.77E-02	0.21	Cosmic Background
3.00E-02	3.00	3.00E+07	1.00E+10	1.00E-02	2.09	4.13E-02	0.48	X-band radar
1.25E-02	1.25	1.25E+07	2.40E+10	2.40E-02	5.03	9.92E-02	1.15	MASER
1.20E-02	1.20	1.20E+07	2.50E+10	2.50E-02	5.24	1.03E-01	1.20	K-band radar
1.00E-03	0.10	1.00E+06	3.00E+11	0.30	62.83	1.24	14.39	millimeter
3.00E-04	0.03	3.00E+05	1.00E+12	1.00	209.44	4.13	47.96	THz
1.57E-04	1.57E-02	1.57E+05	1.91E+12	1.91	400.20	7.90	91.65	Far IR THz
1.00E-04	1.00E-02	1.00E+05	3.00E+12	3.00	628.32	12.40	143.89	Far IR THz
6.82E-05	6.82E-03	6.82E+04	4.40E+12	4.40	921.29	18.18	210.99	First THz QCL
1.57E-05	1.57E-03	1.57E+04	1.91E+13	19.11	4002.04	78.98	916.51	Far IR
1.00E-05	1.00E-03	1.00E+04	3.00E+13	30.00	6283.20	124.00	1.44E+03	CO2 Laser
5.00E-06	5.00E-04	5000.00	6.00E+13	60.00	1.26E+04	248.00	2.88E+03	Mid IR
4.20E-06	4.20E-04	4200.00	7.14E+13	71.43	1.50E+04	295.24	3.43E+03	First QCL
3.00E-06	3.00E-04	3000.00	1.00E+14	100.00	2.09E+04	413.33	4.80E+03	Mid IR
1.30E-06	1.30E-04	1300.00	2.31E+14	230.77	4.83E+04	953.85	1.11E+04	Near IR Fiber
9.80E-07	9.80E-05	980.00	3.06E+14	306.12	6.41E+04	1265.31	1.47E+04	Near IR GaAs
6.80E-07	6.80E-05	680.00	4.41E+14	441.18	9.24E+04	1823.53	2.12E+04	red
4.10E-07	4.10E-05	410.00	7.32E+14	731.71	1.53E+05	3024.39	3.51E+04	violet

Why TeraHertz sources

- Biological agent detection
  - Non-spectroscopic methods are not capable of remote detection of the bio-agent; some contact is required.
    - molecular/DNA based (PCR)
    - immunological
  - Spectroscopic techniques are ideal for remote detection
    - X-rays
      - Wide spread usage (airport scanners, hospitals, etc.)
      - Image mass density (CT, SPECT, PET)
    - Infrared (IR) radiation
      - Absorption of infrared radiation results in vibrational/rotational excitations in organic molecules (FT-IR, FT-Raman)
      - TeraHertz (400-900 cm-1) region is the true fingerprint region and yet it is the least characterized.

Why TeraHertz sources

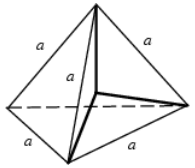
- Nonpolar dry substances like paper, cardboard, thin pieces of wood, and plastic are largely transparent to THz radiation
- TeraHertz radiation is ideally suited to identify water, air voids, and biological agents in sealed packages and containers.

TeraHertz source requirements

- Field Deployable
  - Compact: The source size should be as close as possible to that of the underlying radiation (30 to 300 microns).
  - Low power: The sources should consume a few Watts.
  - Robust: The durability would be best with the following
    - solid-state/semiconductor construction
    - electrically pumped
  - Intense: The sources should emit an average power in the tens of milliWatts range.
  - Tunable: The source should be somewhat flexible in frequency.

Classifying electromagnetic sources

- Most radiation sources fall into these categories
  - Thermal radiators
    - broad-band black-body-like sources
    - intensity weakens beyond mid IR
    - incandescent light bulb (used as sources in FT-IR)
  - Atomic transitions
    - narrow-band sources, not easily tunable
    - operate near optical frequencies
    - gas lamps (neon signs, florescent bulbs) & lasers (HeNe).
  - Molecular excitations
    - inefficient, large, not easily tunable
    - make use of molecular rotations, vibrations, or tunneling
    - CO2 laser, MASER
  - Semiconductor interband transitions
    - very efficient sources
    - mostly limited to mid-IR and above due to band-gap
    - LEDS and laser diodes



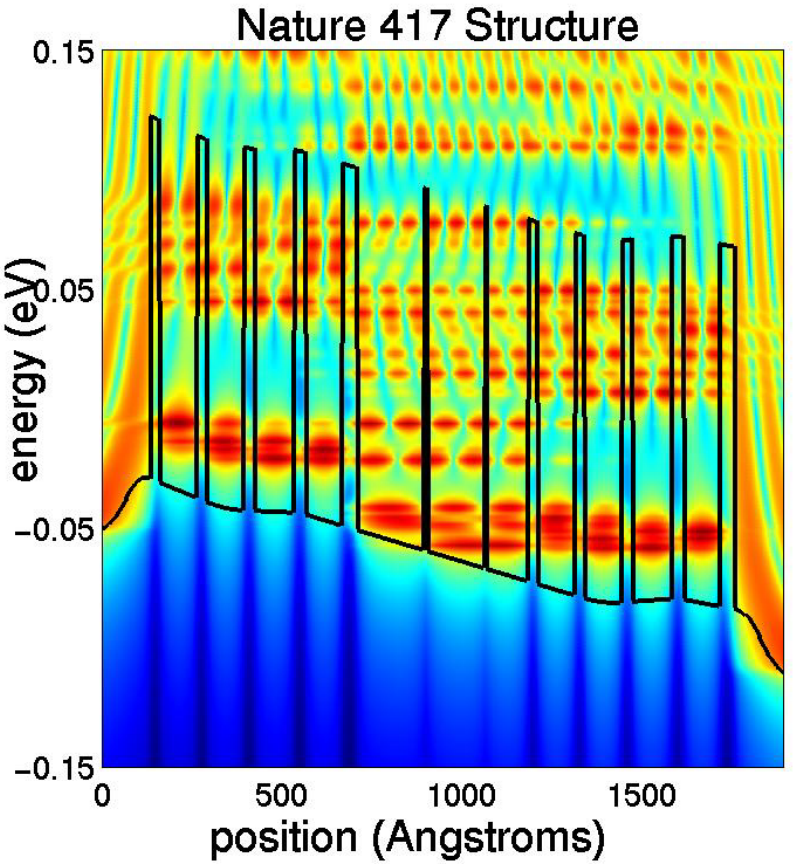
Novel THz sources

- TeraHertz time-domain techniques *
  - Femtosecond laser pulses create photo-generated carriers in a semiconducting material; the transient photocurrent radiates.
  - THz time-domain techniques offer both spectroscopic and imaging
  - Applications include (1) medical (burn severity & cancer diagnosis, cavity detection) (2) Industrial (cracks in composite materials, jet fuel analysis, de-laminations in packaged integrated circuits) (3) Agriculture (water flow analysis in living plants) (4) Environmental protection (gas/pollution detection).
- TeraHertz Quantum Cascade Laser **
  - An integrated solid state component
  - These lasers are the result of sophisticated quantum engineering and semiconductor crystal growth of thousands of layers.
  - The design of the structure determines the emission frequency, not a fundamental property of the bulk material (e.g. the band-gap)
  - The Quantum Cascade Laser approach
    - offers the best chance to satisfy the requirements,
    - and its design requires the simulation of its basic physics.

* Terahertz time-domain spectroscopy probes materials, D. Mittleman, Laser Focus World, 191 (1998)
** Terahertz semiconductor heterostructure laser, R. Kohler et al, Nature **417**, 156 (2002)

Quantum cascade laser

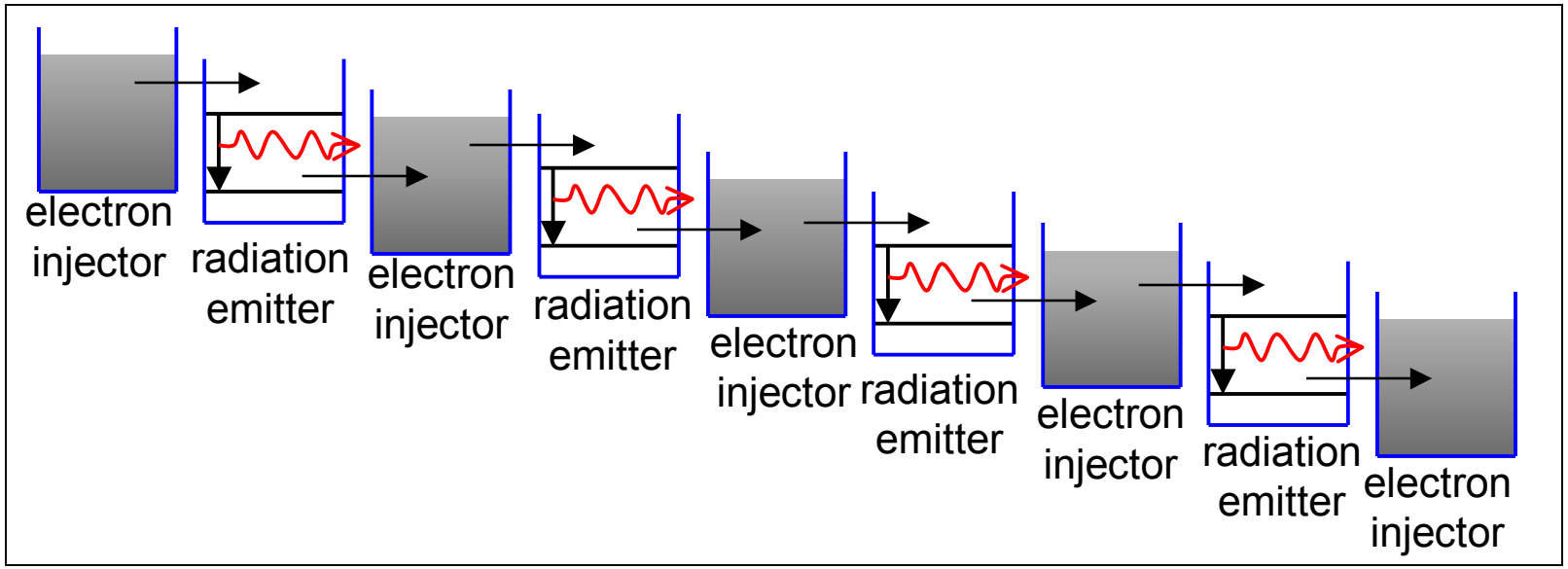
- Progress to date
  - The first QCL was demonstrated in the mid-IR at wavelength of 4.2 microns *
  - The first THz QCL was recently demonstrated in the THz range at 4.4 THz (68 microns) **
- Progress that needs to be made
  - Increasing the output power at sufficiently high temperatures (tens of milliwatts above 80K)
  - Approach CW operation



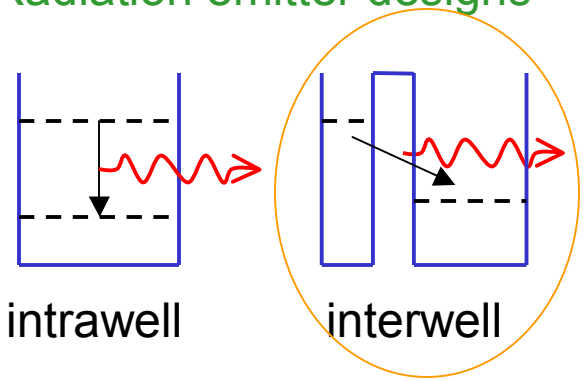
* Quantum Cascade Laser, J. Faist et al., Science **264**, 553 (1994).

** Terahertz semiconductor heterostructure laser, R. Kohler et al, Nature **417**, 156 (2002).

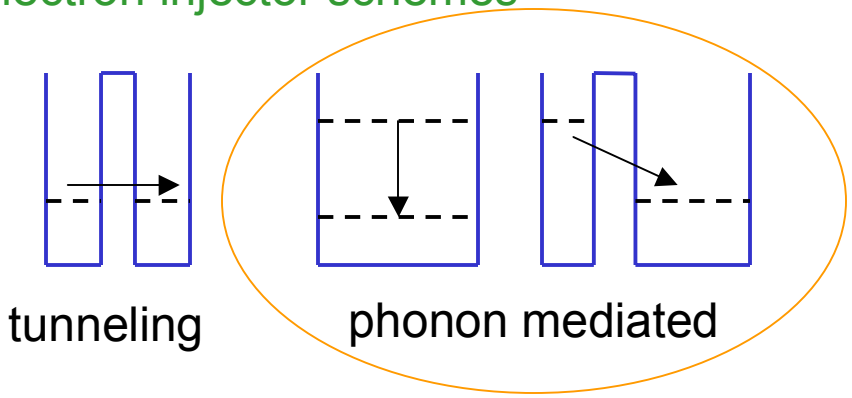
QCL principle of operation



Radiation emitter designs



Electron injector schemes



Cooling requirements

Shallower binding energies act to increase the energy level broadening.

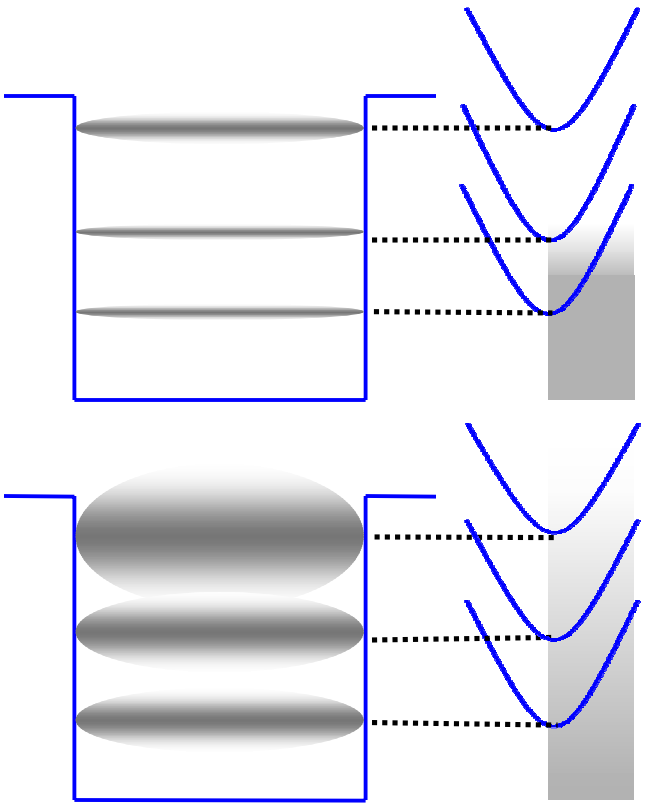
Increased temperatures act to increase the energy level broadening.

$$\tau^{-1} \propto \left(n_b + \frac{1}{2} \pm \frac{1}{2} \right)\left(1 - n_f\right)$$

High temperatures act to equalize the occupancy of the energy levels from a thermal equilibrium viewpoint.

$$\Delta n_f \propto e^{-\Delta E / kT}$$

1.0 TeraHertz = 47 Kelvin
3.0 TeraHertz = 141 Kelvin
4.4 TeraHertz = 211 Kelvin



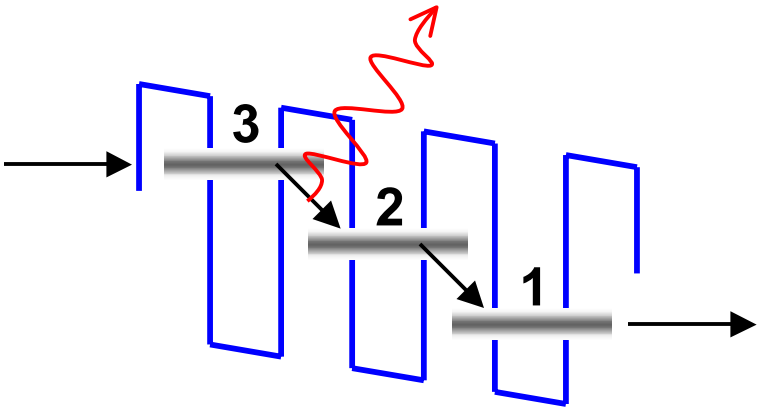
QCL modeling considerations

- A fully self-consistent solution would require a procedure like the following:
  - electrons
    - electron states given the conduction band potential including all scattering processes.
      - Phonon scattering; this will need phonon spectrum
      - Photon scattering
      - Other scattering (e-e)
    - conduction band potential given the charge (electron-states)
  - photons
    - Maxwell equation solution based on the electrons states as source.

- Simplifying assumptions
  - Limit quantum solution to be fully coherent (self-consistent quantum-Poisson), that is no scattering.
  - Include the scattering and coupling to photons, based on the coherent electron states.
  - Use time dependent equation to solve for electron and photon populations; we plan on using the simplest, an empirical rate equation.

Laser Performance Model

Our simulations will be based on a rate equation to model that incorporates the basic physics and ties it together



- Each term describes gain/loss
  - **Electron densities in 3 subbands**
  - **Photon mode density**
  - **Inter-subband scattering times**
  - **Gain, loss, spontaneous emission**

$$\frac{dn_3}{dt} = \frac{J}{e} - \frac{n_3}{\tau_{32}} - \frac{n_3}{\tau_{31}} - gS$$

$$\frac{dn_2}{dt} = \frac{n_3}{\tau_{32}} - \frac{n_2}{\tau_{21}} + gS$$

$$\frac{dn_1}{dt} = \frac{n_3}{\tau_{31}} + \frac{n_2}{\tau_{21}} - \frac{J}{e}$$

$$\frac{dS}{dt} = gS - \alpha S + \beta R_{sp}$$

Electron Energy

- We find the electron energies using quantum mechanics
- Crystal structure needs to be represented
  - We use a generalized Wannier/Bloch function basis to generate a tight-binding electronic structure on a uniform grid.
  - We use the **k·p** method to generate a zone (Γ) centered electronic structure for use on a finite element grid. This method simplifies to a single effective mass conduction band.
  - Effective mass type approximation in both cases.
- Boundary conditions
  - Open boundaries are used for the uniform grid formulation
    - Algebraic linear equation results in continuous eigenvalues.
  - Closed boundaries are used for the finite element formulation.
    - Algebraic generalized eigenvalue equation results in discrete eigenvalues.

Electron Energy

- Self-consistent solution
  - Quantum mechanics
    - input: potential energy of conduction band edge
    - output: wave-function (or equivalent) from which charge can be calculated
  - Gauss Law (or Poisson Equation)
    - input: charge
    - output: potential energy
  - A self-consistent solution is one where a charge and potential satisfy both of the above equations.
  - We use a Newton-Raphson type iteration

Electron energy using a uniform grid

- We model an electron moving in the potential of a lattice under an external field using quantum mechanics
  - Hybrid Wannier/Bloch function representation
    - Bloch function in xy direction
    - Wannier function in z direction
  - We solve an equation based on the single particle Schrodinger equation or a corresponding many electron equation based on second quantization (Dyson's equations).

$$H_0(z) = H^{crystal}(z) + V^{ext}(z), \quad \mathrm{H}^{crystal}(z) = -\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m^*(z)}\frac{d}{dz} + \frac{\hbar^2 k^2}{2m^*(z)}$$

$$\psi(\mathrm{r},t) = \sum_{n\mathrm{k}} f_{n\mathrm{k}}(t)\,\mathrm{w}_n(z)\,e^{i\mathrm{k}\cdot\mathrm{r}} \qquad \Psi(\mathrm{r}) = \sum_{\mathrm{nk}} e^{i\mathrm{k}\cdot\mathrm{r}}\mathrm{w}_{\mathrm{n}}(z)\,a_{\mathrm{nk}}$$

$$i\hbar\frac{\partial\psi(\mathrm{r},t)}{\partial t} = H_0(z)\psi(\mathrm{r},t) \qquad (E - H_0 - \Sigma^{RB})G^{<} = \Sigma^{<B}G^{A}$$

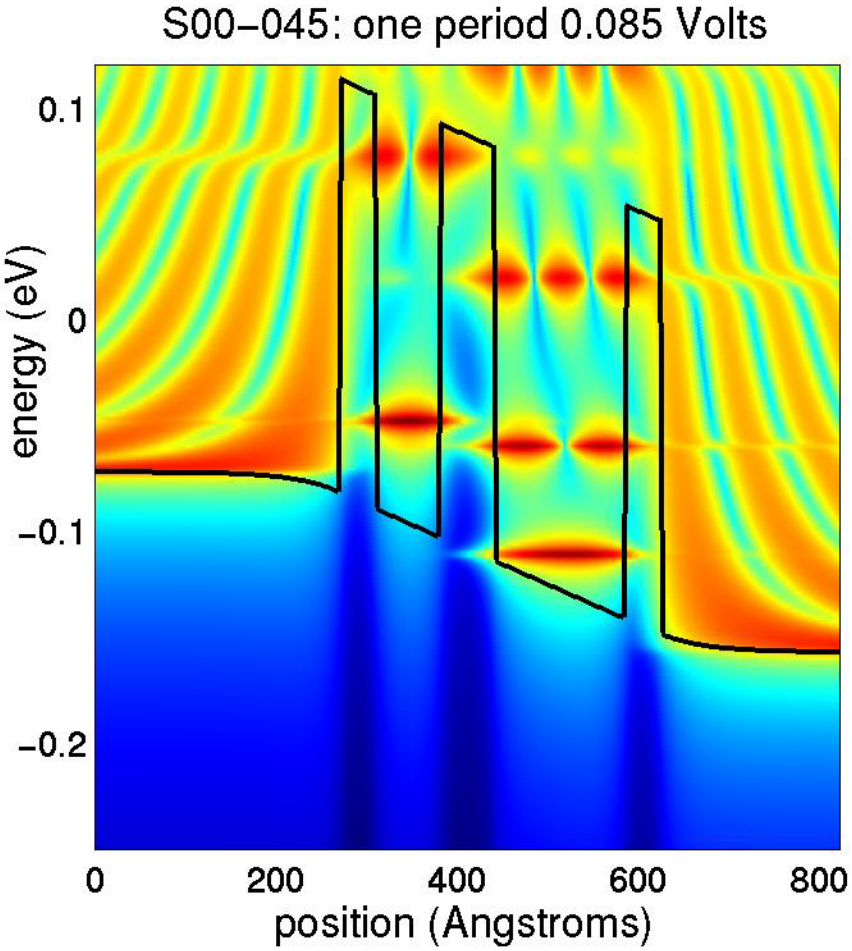
Electron energy using a uniform grid

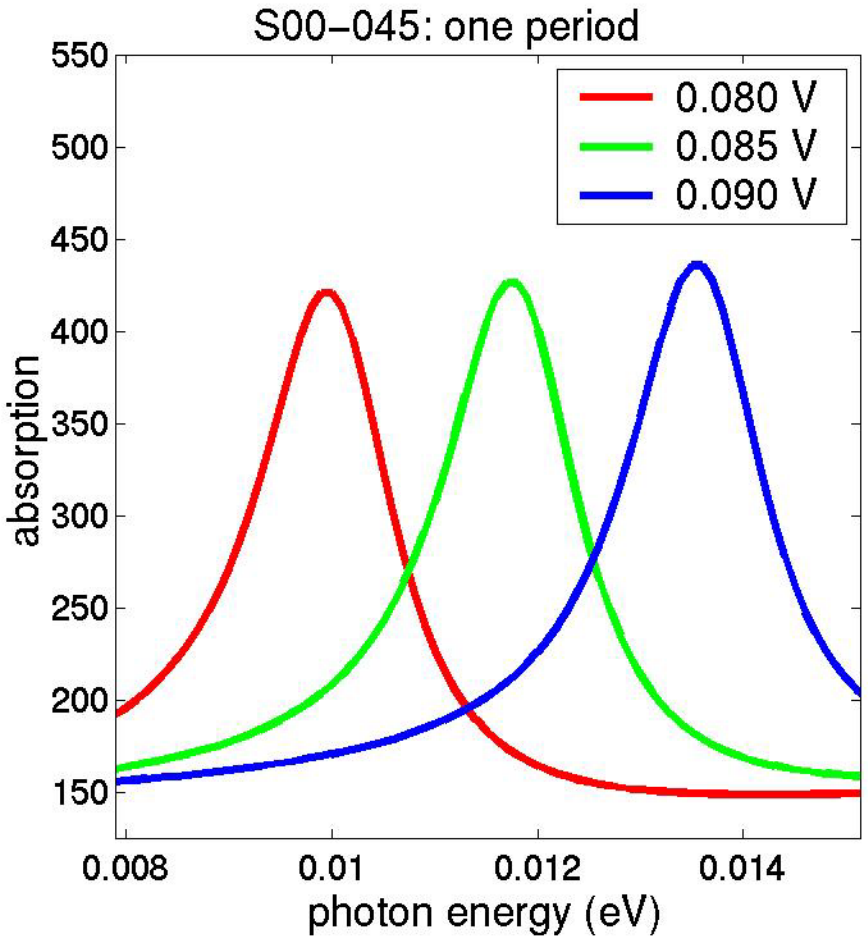
We can calculate the absorption coefficient, $\alpha(\omega)$,which assumes the following form:

$$\alpha(\omega) = \alpha(\mathrm{q} \to 0, \omega)$$

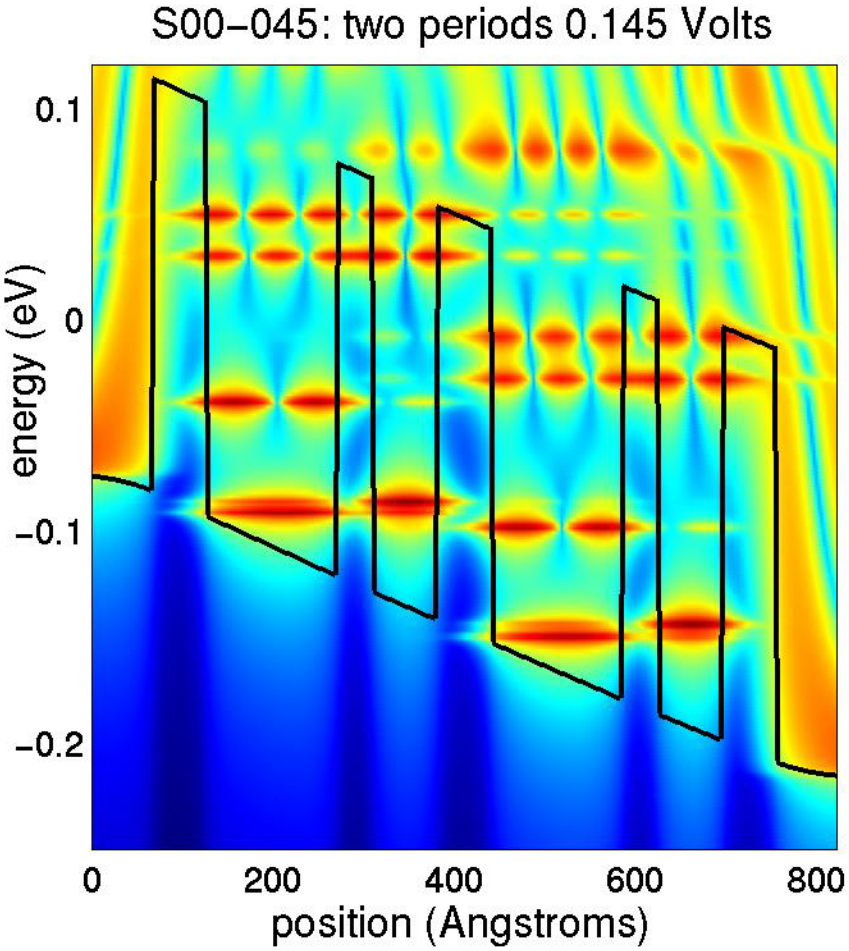
$$\alpha(\omega) \propto \int dE \sum_{mn\mathrm{k}} \begin{bmatrix} -t_{m+1,m} t_{n+1,n} \operatorname{Im} G_{n,m+1}(E) \operatorname{Im} G_{m,n+1}(E+\hbar\omega) \\ +t_{m+1,m} t_{n,n+1} \operatorname{Im} G_{n+1,m+1}(E) \operatorname{Im} G_{m,n}(E+\hbar\omega) \\ +t_{m,m+1} t_{n+1,n} \operatorname{Im} G_{n,m}(E) \operatorname{Im} G_{m+1,n+1}(E+\hbar\omega) \\ -t_{m,m+1} t_{n,n+1} \operatorname{Im} G_{n+1,m}(E) \operatorname{Im} G_{m+1,n}(E+\hbar\omega) \end{bmatrix}$$

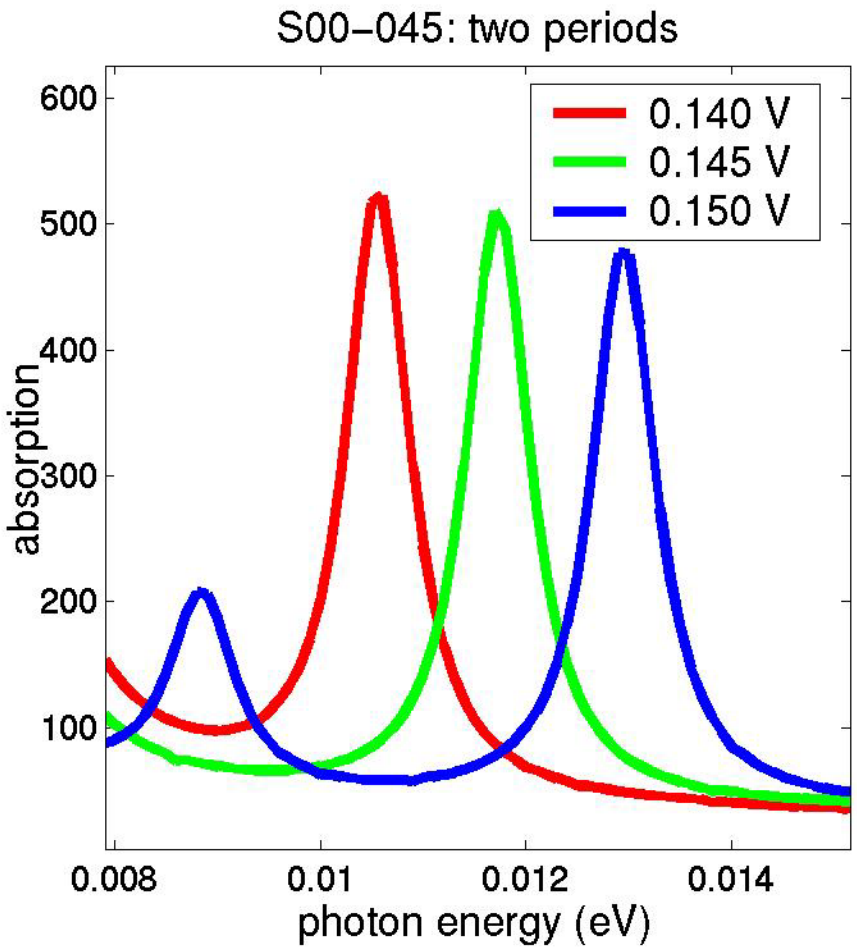
Electron Energy





Electron Energy





Electron energy: new BCs and discretization

- Do we want to simulate this way.
  - Can we lump the continuous levels together?
    - Yes, choose different boundary condition – closed.
  - Are we limited to using a uniform grid?
    - No, but we must choose a different basis for representing the crystal structure – such k·p theory.
    - Use the finite element method

Electron Energy using FEM

The quantum mechanical equation of motion is the Schrodinger equation adapted for use in a layered crystal structure.

$$i\hbar \frac{\partial \psi(\mathrm{r},t)}{\partial t} = -\frac{\hbar^2}{2} \nabla \cdot \frac{1}{m(\mathrm{r})} \nabla \psi(\mathrm{r},t) + V(\mathrm{r},t)\psi(\mathrm{r},t)$$

Finite element analysis based on the Rayleigh-Ritz method requires use of a functional. The desired functional's minimum corresponds to the equation of motion including boundary conditions. The integrand of the functional, L, is the Lagrangian density.

$$L = i\hbar \psi^*(\mathrm{r},t) \frac{\partial \psi(\mathrm{r},t)}{\partial t} - \frac{\hbar^2}{2m(\mathrm{r})} \nabla \psi^*(\mathrm{r},t) \cdot \nabla \psi(\mathrm{r},t) - V(\mathrm{r},t)\psi^*(\mathrm{r},t)\psi(\mathrm{r},t)$$

Electron Energy using FEM

Assume the wave function can be approximated by an expansion over a set of basis functions within each element. We have chosen the simplest, a set of two linear expansion functions.

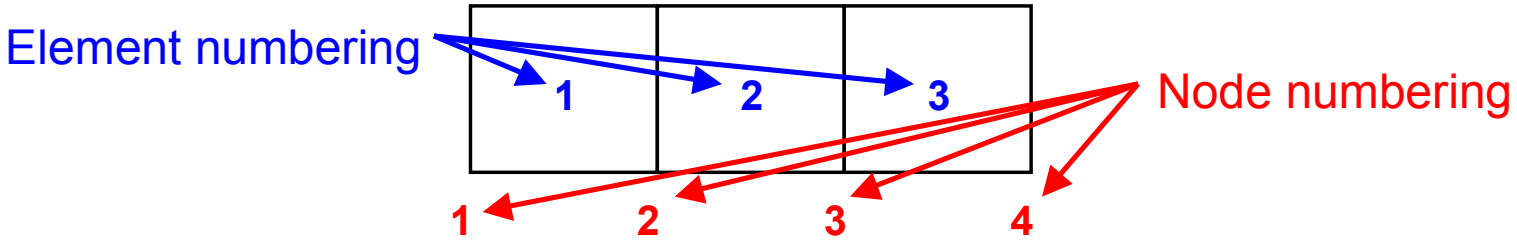
$$\psi(z) = \sum_{i=1}^{2} \psi_i N_i(z), \quad N_1(z) = \frac{z_2 - z}{d}, \quad N_2(z) = \frac{z - z_1}{d}$$

Substitute approximate wave function into functional and minimize by setting its partial derivatives equal to zero

$$\frac{\partial F(\psi_1, \psi_2)}{\partial \psi_i} = 0, \quad F(\psi) = \int dz\, L(\psi)$$

Electron Energy using FEM

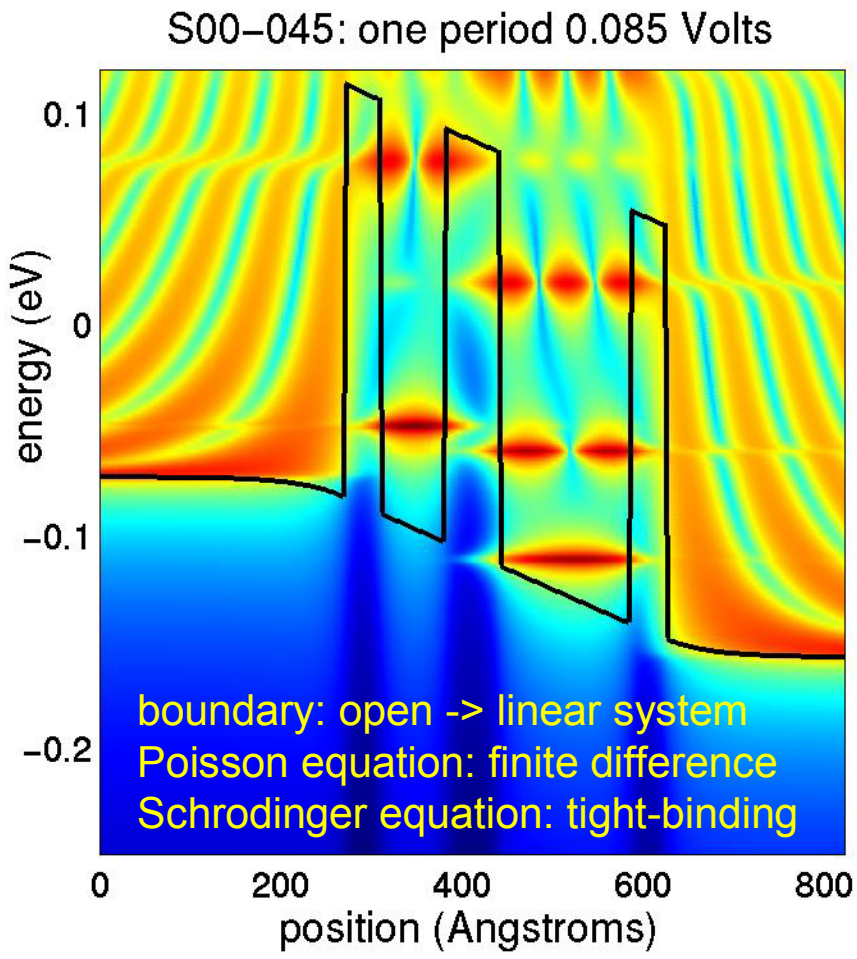
Consider a three element, four node mesh. The matrix equation is of order four, which using the boundary conditions, we reduce by two.

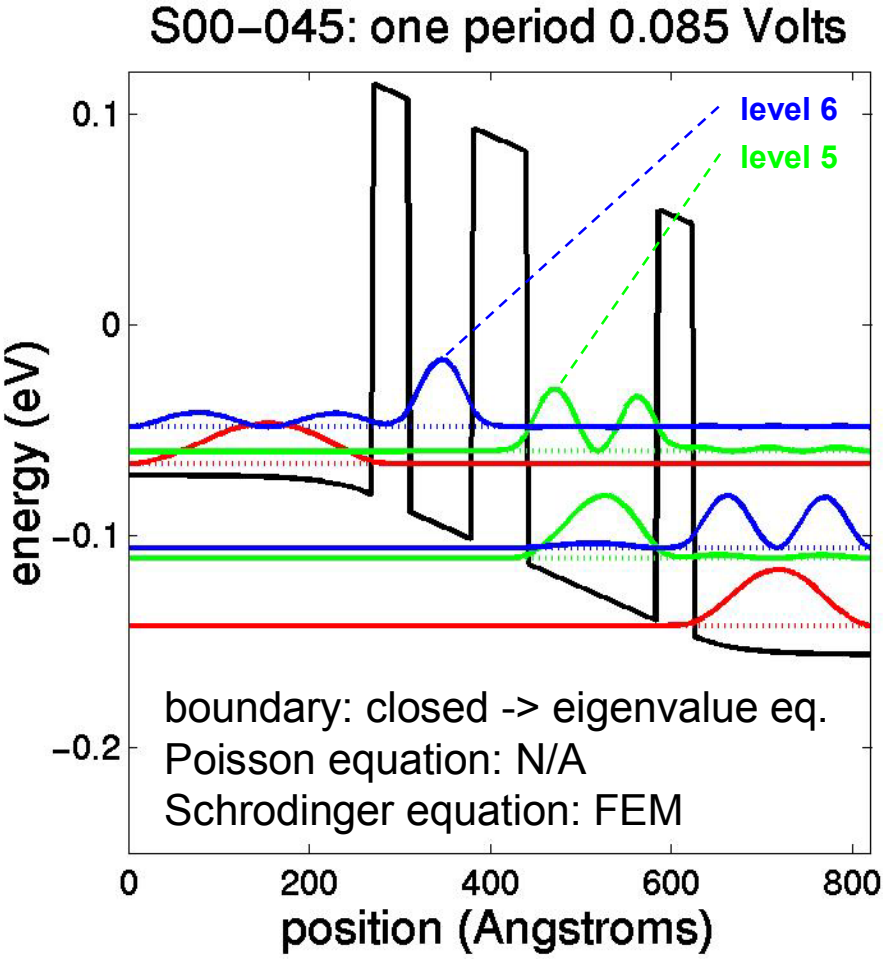


We use Dirichlet boundary conditions such that: $\psi_1 = 0 \quad \psi_4 = 0$

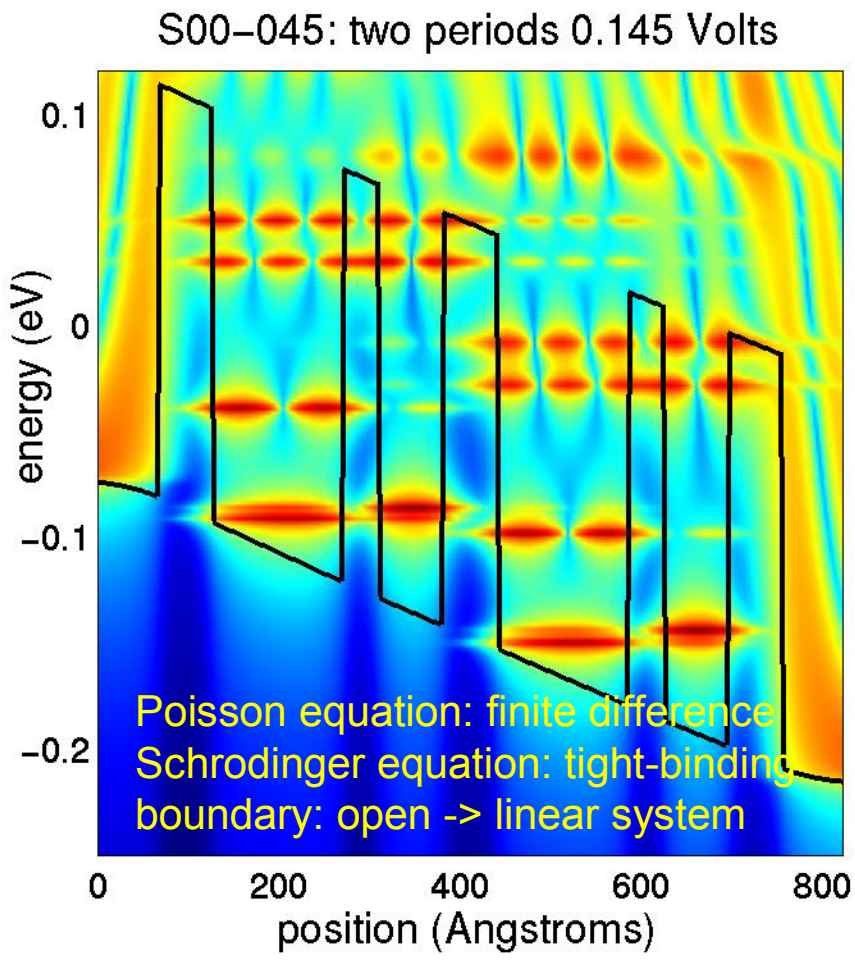
$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{a_1}{h_1}+\frac{b_1 h_1}{3}+\frac{a_2}{h_2}+\frac{b_2 h_2}{3} & \frac{-a_2}{h_2}+\frac{b_2 h_2}{6} & 0 \\ 0 & \frac{-a_2}{h_2}+\frac{b_2 h_2}{6} & \frac{a_2}{h_2}+\frac{b_2 h_2}{3}+\frac{a_3}{h_3}+\frac{b_3 h_3}{3} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} - E \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{h_1}{3}+\frac{h_2}{3} & \frac{h_2}{6} & 0 \\ 0 & \frac{h_2}{6} & \frac{h_2}{3}+\frac{h_3}{3} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

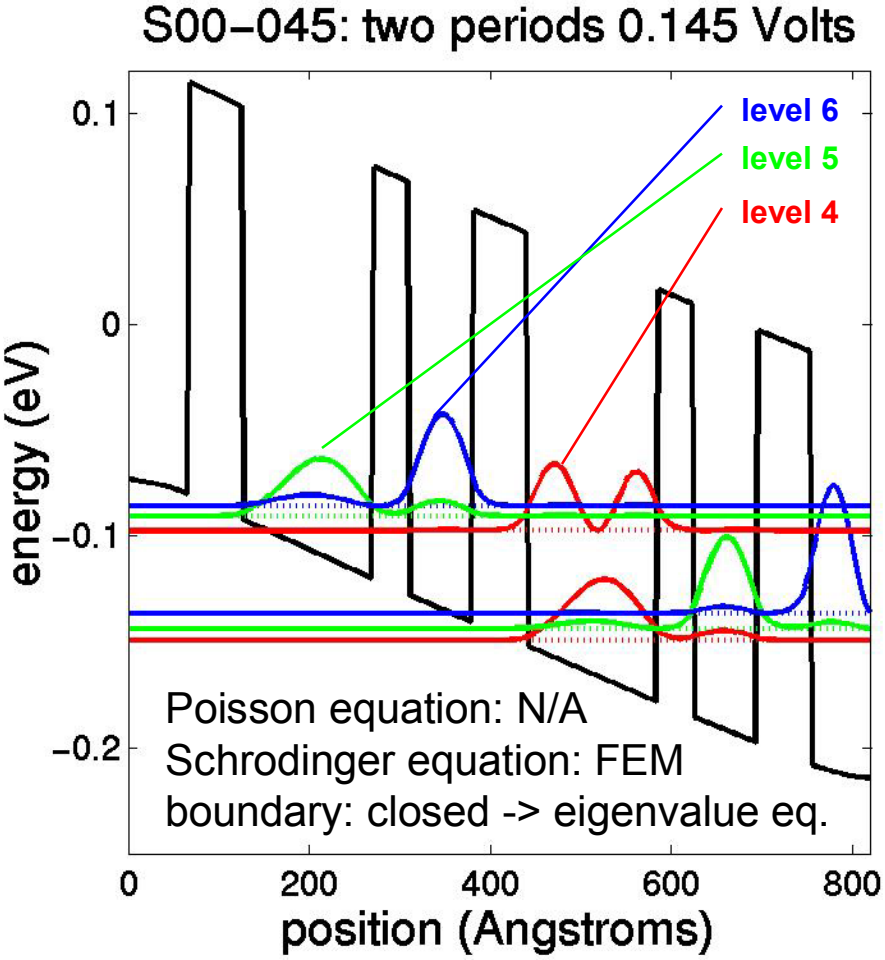
Electron Energy: FEM Results



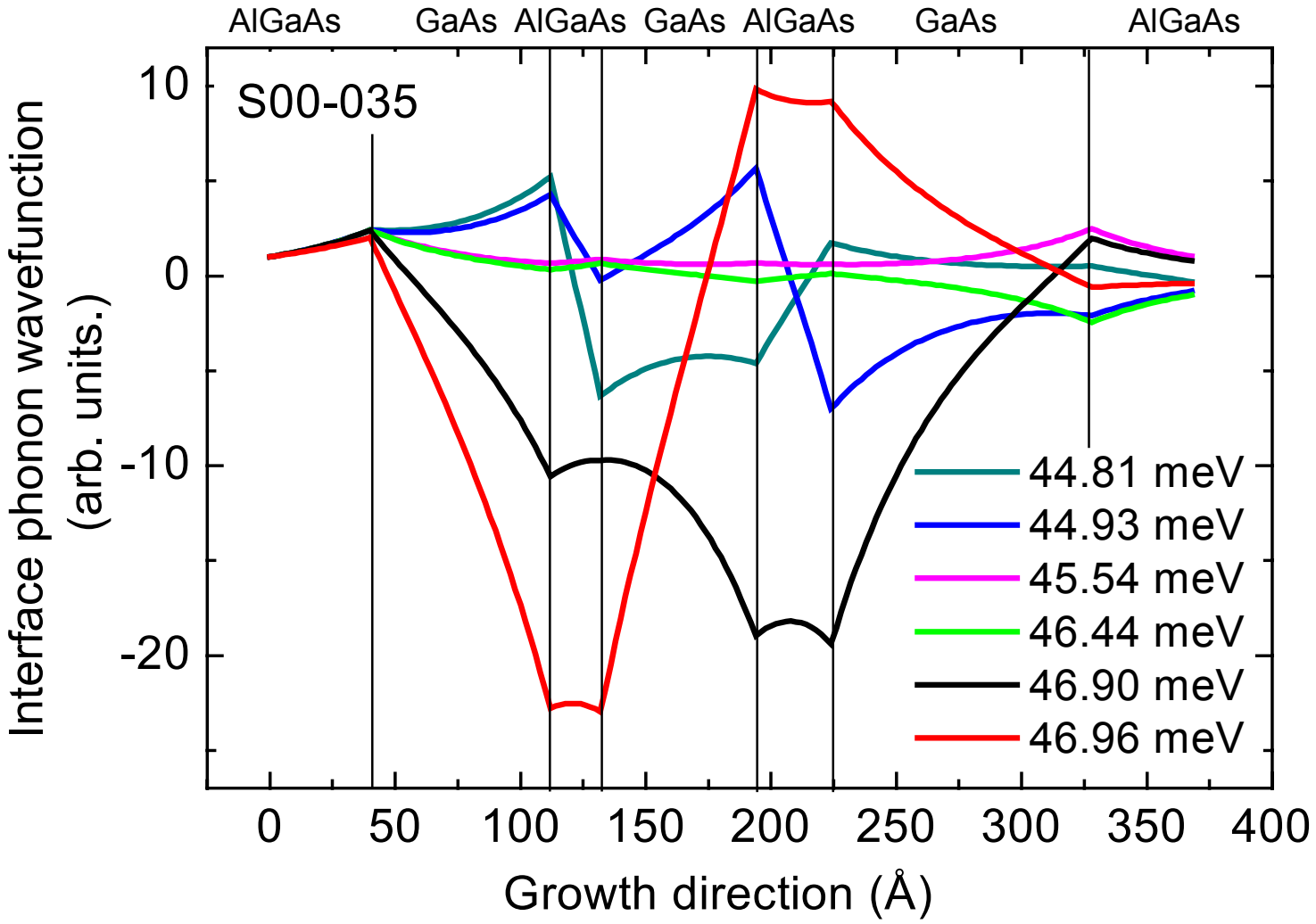


Electron Energy: FEM Results

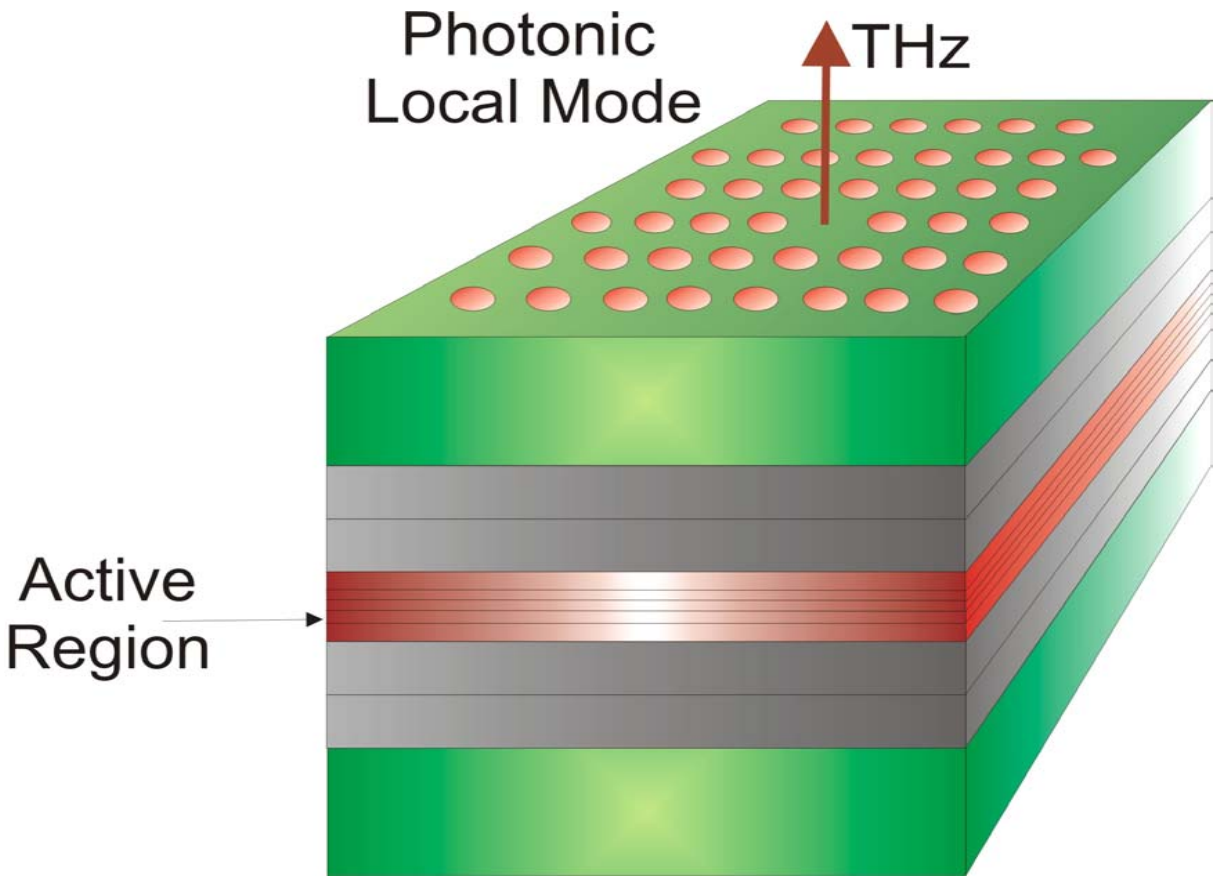




Interface Phonon Energies



Optical Cavity



Find Optimum Device

- We will apply global optimization techniques to intelligently extract the best device structure from a computationally driven statistical sample of devices.
  - based on the laser's essential physics because we will use cost functions that are based on the rate equation's solution.
  - The statistical sample of structures will have layers that vary in thickness and in terms of the stoichiometric ratio (x) of the barrier's material composition which is Ga(1-x)Al(x)As.
  - An optimum structure will be one that is best in one or more characteristics, while constrained in other characteristics. A relevant example optimum structure could be one that emits at the highest possible intensity, while operating near a target wavelength (3 THz) with a given tune-ability (10%), and having a certain cooling requirement (77 K).
- High Performance Computing is necessary due to the large parameter space of the search
  - We will explore parallelization opportunities in the optimization as well as in the eigenvalue problem.

Software design considerations

- Standard C++ ISO/IEC 14882-1998
  - Object oriented
    - Abstraction (accessing data through well defined interfaces)
      - We access data through member functions.
    - Encapsulation (enforcing the hiding of implementation details)
      - We generally keep data members private.
      - We make use of friend classes.
    - Hierarchy (composition and derivation encourages code re-use)
      - We use classes that use both composition and derivation
      - We use templates to share the same code for double and complex
      - We use template specializations when different code is necessary
    - Polymorphism (the same code works for different objects)
      - We make use of virtual functions and base class pointers

Software design considerations

- Standard C++ ISO/IEC 14882-1998
  - C++ is a compiled language
    - Standard optimization techniques
    - Access to system resources (e.g. memory limits)
  - Parallelism is supported through standard libraries (e.g. MPI, Pthreads) as well as other standards (OpenMP).
  - C++ source can be portable
    - Compiled by “gmake” on SunOS, AIX, IRIX64
    - Use of the C++ Standard Library (iostream, fstream, vector, valarray, and complex)
  - Interfaces well with C and Fortran

Summary

- This is a new project; it is a few months old.
- It is a collaboration between DoD and academia.
- TeraHertz radiation
  - is ideally suited to identify water, air voids, and biological agents in sealed packages and containers.
  - nonpolar dry substances like paper, cardboard, thin pieces of wood, and plastic are largely transparent to THz radiation
- The Quantum Cascade Laser approach
  - offers the best chance to satisfy the requirements,
  - and its design requires the simulation of its basic physics.
- Simulation strategy requires high performance computing
- We have some initial computational results